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The Effect of Curvature on Detonation Speed

Bruce Bukiet

Research and Development Report

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The Effect of Curvature on Detonation Speed

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ABSTRACT

This is the second in a series of papers describing a program for the numerical modelling of detonation waves. In this paper, we establish the validity of an asymptotic theory, developed by J. Jones, for the correction to detonation wave speed due to the curvature of an expanding cylindrically symmetric detonation wave. We take as a test problem an expanding cylindrically symmetric CJ detonation wave. A random choice computation in which the reaction zone is resolved and in which operator splitting is applied to both the geometrical source terms and the chemical source terms is used to solve this problem. The solution by this method on a fine grid is taken as exact. The solution using the quasi steady state theory of Jones is also applied to this problem. It is shown numerically that Jones' equations supply the correction to wave speed due to the curvature of the front to first order in the inverse of radius.

This result, in combination with the result of the previous paper in this series, will enable the computation of the transition from strong detonations to weak detonations of two dimensional curved detonations using the front tracking method in the near future.

1. Introduction

A basic problem in the theory of detonation has been to understand the transition from strong to weak detonations caused by an expanding geometry. In this and related and forthcoming papers, we show that the theory of Jones [10] provides a solution to this problem

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[2] Supported in part by the Army Research Office, grant DAAG29-85-K0188.

through first order in inverse radius of curvature. Moreover, we use this knowledge to provide a method for the computation of detonations which appears to show consderable promise.

In this paper, we study the influence of the radius of curvature on the speed of a cylindrically expanding detonation wave with finite reaction rate. We also study the effect of curvature on the reaction zone. The central issue to be analyzed is the consequence of radially induced cooling on the chemical reaction. See [7] for a review of this topic and more generally of the theory of detonations in the presence of endothermic effects.

Two numerical methods are used to solve this problem. First, a one dimensional random choice computation with operator splitting for both the radial effects and the effects of the finite reaction rate is employed. Since this method resolves the reaction zone numerically (in contrast to [2]), it includes curvature effects on the detonation velocity. This method gives an accurate solution for grids fine enough to capture the dynamics within the reaction zone. Next, we discuss recent contributions by J. Jones [10], who derived a system of quasi steady state ordinary differential equations to describe expanding detonations. We solve these equations numerically to find the wave speed and to resolve the reaction zone. The solutions of Jones' equations are found to be correct to first order in powers of inverse radius thereby confirming and validating his analysis.

A motivation for this work was to enhance the front tracking algorithm (see [3]) to allow calculation of curvilinear detonation fronts in their transition from strong to weak detonations.

2. The Random Choice Computation

In this section, we discuss the solution to the equations of reactive gas dynamics with finite reaction rates in a symmetric geometry. The Zeld'ovich-Von Neumann-Doering (ZND) model of detonations (see [7]) is used. For this model, the equations of inviscid gas dynamics with cylindrical symmetry become

$$\mathbf{w}_t + \mathbf{f}(\mathbf{w})_r = \mathbf{C} - \alpha \mathbf{G} \ , \tag{2.1}$$

where

$$\mathbf{w} = \begin{pmatrix} \rho \\ m \\ e \\ \lambda \end{pmatrix} \qquad \mathbf{f}(\mathbf{w}) = \begin{pmatrix} m \\ \dfrac{m^2}{\rho} + P \\ \dfrac{m}{\rho}(e+P) \\ m\dfrac{\lambda}{\rho} \end{pmatrix} ,$$

$$\mathbf{C} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ R(\lambda,T) \end{pmatrix} \qquad \mathbf{G} = \begin{pmatrix} \dfrac{m}{r} \\ \dfrac{m^2}{\rho r} \\ \dfrac{m}{\rho r}(e+P) \\ 0 \end{pmatrix} ,$$

and

$$\alpha = \begin{cases} 0 & \text{for planar geometry} \\ 1 & \text{for cylindrical geometry} \\ 2 & \text{for spherical geometry} \end{cases} .$$

$\mathbf{C}$ and $\alpha\mathbf{G}$ are respectively, the source terms due to combustion and geometry. In these equations, ρ is the density of the gas, m is the momentum density, P is the pressure and λ is the mass fraction of burned gas ($0 \le \lambda \le 1$). The energy per unit volume, e, may be written as

$$e = \rho\epsilon + \frac{\rho u^2}{2}$$

where u is the velocity and ϵ is the specific internal energy. Assuming a polytropic equation of state,

$$\epsilon = \frac{P}{\rho(\gamma-1)} + (1-\lambda)q ,$$

with $\gamma > 1$. In order to simplify the formulas, the polytropic constant, γ, is assumed to have the same value in the unburned, burned and reacting gas. The heat released during combustion is q; T is the temperature ($T = P/\rho$) and $R(\lambda,T)$ is the reaction rate. We use Arrhenius kinetics, which yields an infinite reaction length. Thus,

$$R(\lambda,T) = \begin{cases} k(1-\lambda)\exp\left(-\frac{E}{T}\right) & , T \geq T_c \\ 0 & , T < T_c \end{cases}$$

where k is the rate multiplier, and E is the activation energy. We introduce T_c, the critical temperature below which the reaction rate is taken to be identically zero, in order to allow for quenching and to eliminate the cold boundary effect. That is, if there were no critical temperature, the reaction rate would be positive even for cold gases. Then, the unburned gas would begin to burn before the shock wave encountered it.

To solve this system numerically, we employ operator splitting [12]. At the start of a time step, we solve the homogeneous system

$$\mathbf{w}_t + \mathbf{f}(\mathbf{w})_r = 0 \tag{2.2}$$

by the random choice method [9],[4]. The Newton's method of [2] is employed to solve the Riemann problems that arise in this computation. Next, we use the solution of eq. (2.2) as initial data for the system of ordinary differential equations for the geometrical source terms,

$$\mathbf{w}_t = -\alpha\mathbf{G}\ , \tag{2.3}$$

Finally, we use the solution of eq. (2.3) as initial data to solve

$$\mathbf{w}_t = \mathbf{C},$$

the equation for the source term due to chemistry. This sequential operator splitting calculation converges under mesh refinement. Colella, Majda and Roytburd [5] have used a three part splitting in their fractional step method computations for reacting gases.

A plot of pressure vs. distance for a stable planar reaction is shown in Fig. 2a at the start of a calculation, initialized with the steady state solution, and after several hundred time steps using the method described above. In addition, reactions which have parameters chosen to yield unstable detonations are modelled well by this method. In an example of an unstable detonation, our results agree with those of Erpenbeck [6] , Mader [11] and Fickett and Wood [8] (see Fig. 2b).

We note that when performing these calculations one must take care not to introduce spurious effects due to the numerical modelling techniques. In modelling the reaction zone accurately, one should include enough grid points in the region of significant chemical activity. We suggest using at least 20 computational zones in the region between the shock which initiates the reaction and the point at which 90% of the gas is burned. However, in order to eliminate any possible uncertainty from our one dimensional computations, much finer grids were employed. Another consideration comes into play as the reaction progresses, namely that the region of chemical activity grows in time for the Arrhenius model of kinetics. To deal with this problem, we eliminate the portion of the computational region more than a certain distance behind the initiating shock wave. In doing so, care must be taken to eliminate only regions in which there are very small variations in the gas states. Introducing even weak waves into the reacting gas in this elimination process is equivalent to releasing small amounts of energy on a slow time scale and can cause large errors. This phenomenon was studied by Bdzil [1].

3. The Asymptotic Method of Jones

In [10], J. Jones derived and analyzed a method of calculating the effect of curvature on the speed of an expanding cylindrical or spherical detonation wave to first order in powers of the inverse of radius of curvature. This theory also predicts the state of the gas through the reacting region.

The radius of curvature of the detonation wave is assumed to be much larger than the length of the reaction zone. In the case of Arrhenius kinetics, as considered here, the reaction zone length may be defined, for example, as the distance from the initiating shock wave to the point at which 90% of the gas is burned. It is also assumed that the reaction has proceeded for many reaction zone lengths so that initial transients are eliminated. Thus the run has settled down to a quasi steady state. Further, the state of the unburned gas ahead of the shock is constant with zero velocity. Through the methods of perturbation theory, eliminating higher order terms, Jones derived the following system of ordinary differential equations from eq. (2.1):

$$u_x = \frac{q(\gamma - 1)k(1 - \lambda)\exp\left(-\frac{E\gamma}{c^2}\right) - \frac{uc^2}{z}}{(\dot{z} - u)^2 - c^2} \tag{3.1}$$

$$\lambda_x = \frac{R(\lambda, T)}{\dot{z} - u}$$

$$c^2 = c_o^2 + \frac{\gamma - 1}{2}(\dot{z}^2 - (\dot{z} - u)^2) + q(\gamma - 1)\lambda$$

where c_o represents the sound speed in the unburned gas ahead of the shock, c is the speed of sound of the reacting gas, $c = \left\{\gamma P/\rho\right\}^{\frac{1}{2}}$, x is the distance behind the initiating shock wave, z is the radius of curvature of the shock, and $\dot{z}$ is the wave speed.

In the case of an undriven planar detonation, the reaction terminates at the Chapman-Jouguet (CJ) point on the Hugoniot curve. This is a sonic point. That is, a point at which the wave moves at sound speed with respect to the gas behind it. However, an expanding detonation is weakened by expansion induced rarefactions coming from behind the shock and the termination point for the reaction moves below the CJ point yielding a weak detonation. The flow is subsonic behind a shock but supersonic behind a weak detonation. Thus, a transition from subsonic to supersonic flow must occur in the reacting gas.

Since the denominator of the first of eqs. (3.1) vanishes at any sonic point, in order to have a smooth transition through a sonic point, the numerator must also vanish there. The transformation

$$y \equiv \int^{x} \frac{dx'}{c(x')^2 - v(x')^2}$$

where $v = \dot{z} - u$, leads to the system

$$(3.2) \qquad v_y = q(\gamma - 1)k(1 - \lambda)\exp\left(-\frac{E\gamma}{c^2}\right) - \frac{\dot{z} - v}{z}c^2$$

$$\lambda_y = \frac{1}{v}k(1 - \lambda)\exp\left(-\frac{E\gamma}{c^2}\right)(c^2 - v^2)$$

where

$$c^2 = c_a^2 + \frac{\gamma - 1}{2}(\dot{z}^2 - v^2) + q(\gamma - 1)\lambda .$$

This transformation does not change the structure of the phase plane and the critical point conditions for this system are the same as the conditions for a smooth sonic transition mentioned above. These conditions are:

$$(3.3) \qquad q(\gamma - 1)k(1 - \lambda)\exp\left(-\frac{E\gamma}{c^2}\right) - \frac{\dot{z} - v}{z}c^2 = 0$$

$$\frac{1}{v}k(1 - \lambda)\exp\left(-\frac{E\gamma}{c^2}\right)(c^2 - v^2) = 0$$

$$c_a^2 + \frac{\gamma - 1}{2}(\dot{z}^2 - v^2) + q(\gamma - 1)\lambda = c^2 .$$

From a computational point of view, eqs. (3.2) are easier to work with than eqs. (3.1), see also [10].

We know the state of the gas ahead of the shock wave which initiates the reaction as well as the radius of curvature of this wave. We also know that the wave speed, $\dot{z}$, must be at least as large as the sound speed of the ahead state since the flow ahead of a shock wave is supersonic. In addition, the wave speed is no more than the speed of a planar Chapman-Jouguet detonation since it is undriven and weakened by the expansion. Hence, we have a range of possible values of $\dot{z}$ and thus also of v immediately behind the shock, which we refer to as v_0. To solve for the wave speed and resolve the reaction zone we proceed as follows. We guess a value for v_0 and solve for the critical point of the system of ordinary differential equations (3.2) by iterating on λ and v, using the equations

$$v = \left\{ \frac{2}{\gamma + 1} \left(c_a^2 + \frac{(\gamma - 1)\,\dot{z}^2}{2} + q(\gamma - 1)\lambda \right) \right\}^{\frac{1}{2}}$$

$$\lambda = 1 - \frac{(\dot{z} - v)\, c^2 \exp\left(\frac{E\gamma}{c^2} \right)}{qk(\gamma - 1)z}$$

which are derived from eqs. (3.3), using the fact that $v^2 = c^2$ at the sonic point. The square root takes the same sign as $\dot{z}$. We then integrate system (3.2) numerically with the initial conditions

$$v(0) = v_0$$

$$\lambda(0) = 0$$

to find the trajectory of the solution in the $v - \lambda$ plane for the given $\dot{z}$. We update the values of v_0 and $\dot{z}$ based on this trajectory by a bisection method until the trajectory passes within a specified tolerance of the critical point. The solution is continued through the critical point by finding the eigenvectors there. The equation, see [10],

$$p_x = -\rho v v_x$$

and the last of eqs. (3.2) are used to compute the pressure and density through the reacting region.

In Fig. 3a, we present the $v-\lambda$ phase plane portrait as well as the sonic locus for the value of $\dot{z}$ which yields a sonic transition for the given data. The curve passes through the critical point (S) after which the burning continues on the supersonic side of the sonic locus.

4. Results

In Fig. 4a, we compare a plot of the pressure, immediately behind the shock wave which initiates the detonation, vs. time for a planar CJ detonation, computed by the random choice method described in §2 ($\alpha = 0$), with a plot of the results from a cylindrical computation ($\alpha = 1$) and with the results of the method of Jones where the radius of curvature is assumed to be the same as for the cylindrical computation at all times. The vertical error bars give the highest and lowest values of pressure over each 100 time steps for the random choice computations. As expected, the pressures computed by the two cylindrical methods approach the planar CJ pressure just behind the shock as the radius of curvature increases. We note that the random choice computations are initialized with the planar steady state solution and it takes some time for the initial transients to disappear in the cylindrical run. When we initialized the random choice method with the results of Jones' method at a small radius the transients were much smaller but the results for larger radii were not significantly different from those of the planar initialization. A comparison of the pressures behind the shock wave using these initializations is seen in Fig. 4b. In these computations, we eliminated the regions more than 3 reaction zone lengths behind the initiating shock wave.

To exhibit the validity of Jones' method to leading order in inverse radius, we present, in Fig. 4c, a plot of pressure behind the initiating shock wave vs. inverse radius for the numerical methods described in §2 and §3. We also show the line predicted by the theory of Jones for the leading order corrections to pressure due to curvature, based on computations using Jones' equations with very large radius of curvature. The oscillations in the random choice computation are due to the numerical method and decrease with refinement of the grid. A similar plot is achieved for the corrections of detonation wave speed due to curvature (Fig 4d). We note that the leading order of Jones' theory is much more accurate than the full Jones' theory, indicating the presence of spurious R^{-2} terms in the full theory.

Fig. 4e shows the states of a reacting gas for a planar CJ detonation, for an expanding cylindrical detonation using the method described in §2, and for the method of Jones at a fixed time. We have plotted pressure vs. specific volume along with the unburned and burned Hugoniot curves. It is plotted at a time when the radius of curvature is approximately 50 times the length of the reaction zone. The steady state planar wave is initiated by a shock and moves down the Rayleigh line from A to CJ (the CJ point) as the reaction progresses. This line, when extended, passes through the point representing the initial ahead state. The detonation waves for the two cylindrical methods are initiated by weaker shocks, corresponding to a lower pressure on the unburned Hugoniot (points F and D), and move down along the curves shown to a weak detonation. These curves do not terminate on the burned Hugoniot curve since it is computed from a planar theory. Wood and Kirkwood [13] have derived equations for the modifications of Hugoniot curves in a curved geometry. From Fig. 4e, we see the effect of curvature on the pressure just behind the shock and through the reaction zone. These computations show that a 12.5-17.5% smaller jump in pressure at the shock occurs in the curved geometry than in the corresponding planar calculation. Here the radius of curvature was approximately 50 times the reaction zone width.

5. Conclusions

We have shown that the derivation by J. Jones [10] of the corrections due to curvature of the speed of detonation waves and the pressure behind the shock wave are correct to first order in the inverse of radius of curvature. This validation was necessary since the passage from the original system of partial differential equations (2.1) to the ordinary differential equations (3.2) has not been shown rigorously. A rigorous derivation of the equivalence of these two systems would be a significant undertaking.

The advantage of using the equations of Jones is considerable. Solving for the wave speed and the states of the reacting gas is usually accomplished in less than 10 CPU seconds on the ELXSI. We note that the rapid computation of wave speeds will enable two dimensional front tracking computations to be extended to include the effects of curvature on detonation waves in the near future. Although not directly comparable, the one dimensional computations with fully resolved chemical reactions, fine grids and Arrhenius kinetics, exhibited in Figs. 4a-e, require approximately 40 hours of CPU time on the same machine. To avoid these slow computations, for practical computations one would normally use neither resolved chemical reactions, nor fine grids, nor Arrhenius kinetics. The comparison of computations based on Jones' equations with faster but under-resolved computations would involve possible improvements in accuracy as much as speed. It would be desirable to carry out such comparisons.

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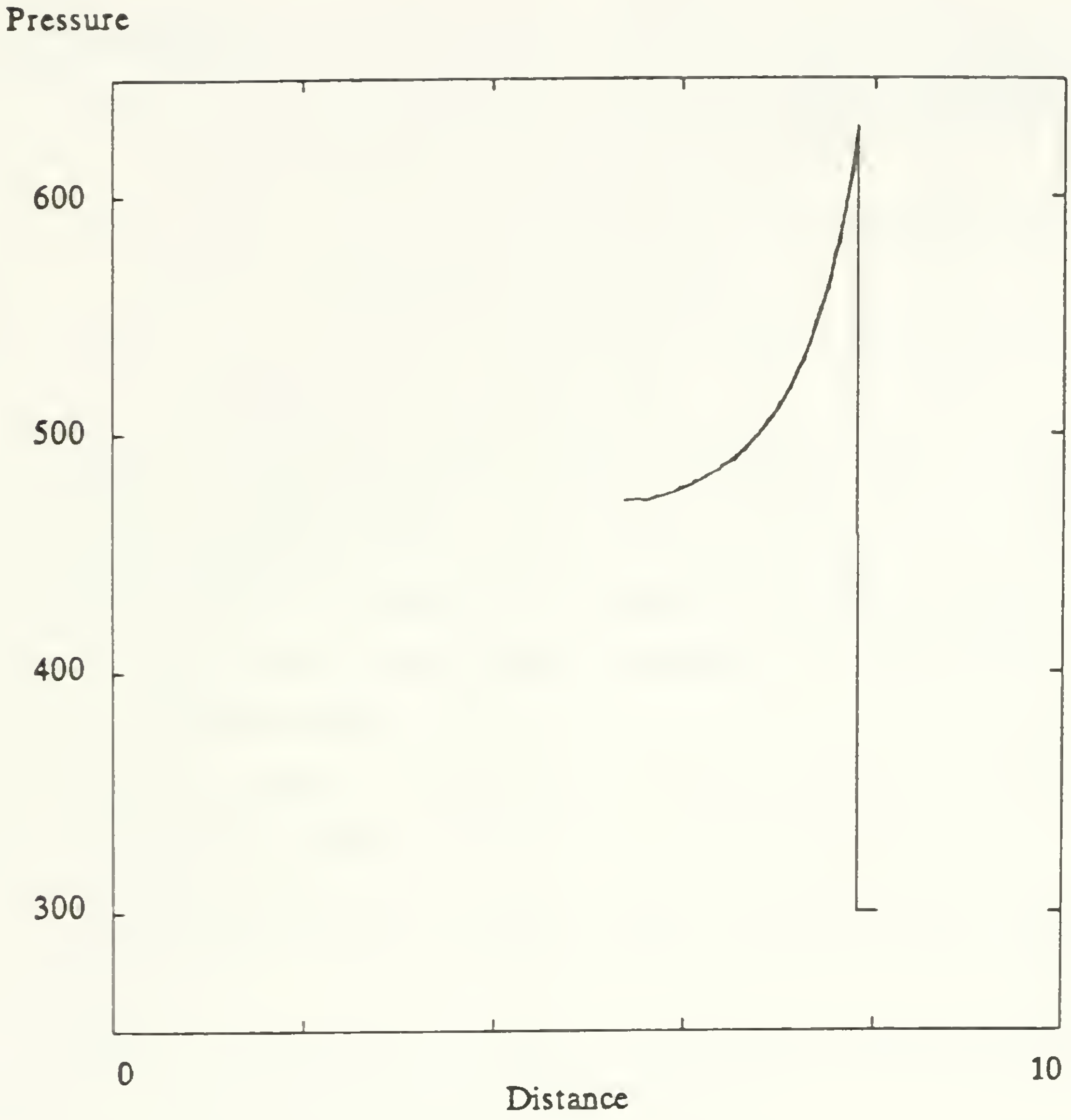

Fig. 2a. A 1D Stable Computation. *A plot of pressure vs. distance is shown for a planar detonation initialized with the steady state ZND solution. The initialized reaction and the reaction 1200 time steps later are superimposed so that both fronts are at the same location on the graph. The solution is clearly not deformed by the numerical method. The state ahead of the initiating shock (in units where the gas constant $R = 1$) has $P = 100$, $u = 0$, $\rho = 1.4$. The heat release ,q, is 300; $E = 100$; $T_c = 215$ and $\gamma = 1.1$. The distance from the initiating shock wave to the point where the gas is 90% burned is 0.75 and the grid spacing is 0.0125.*

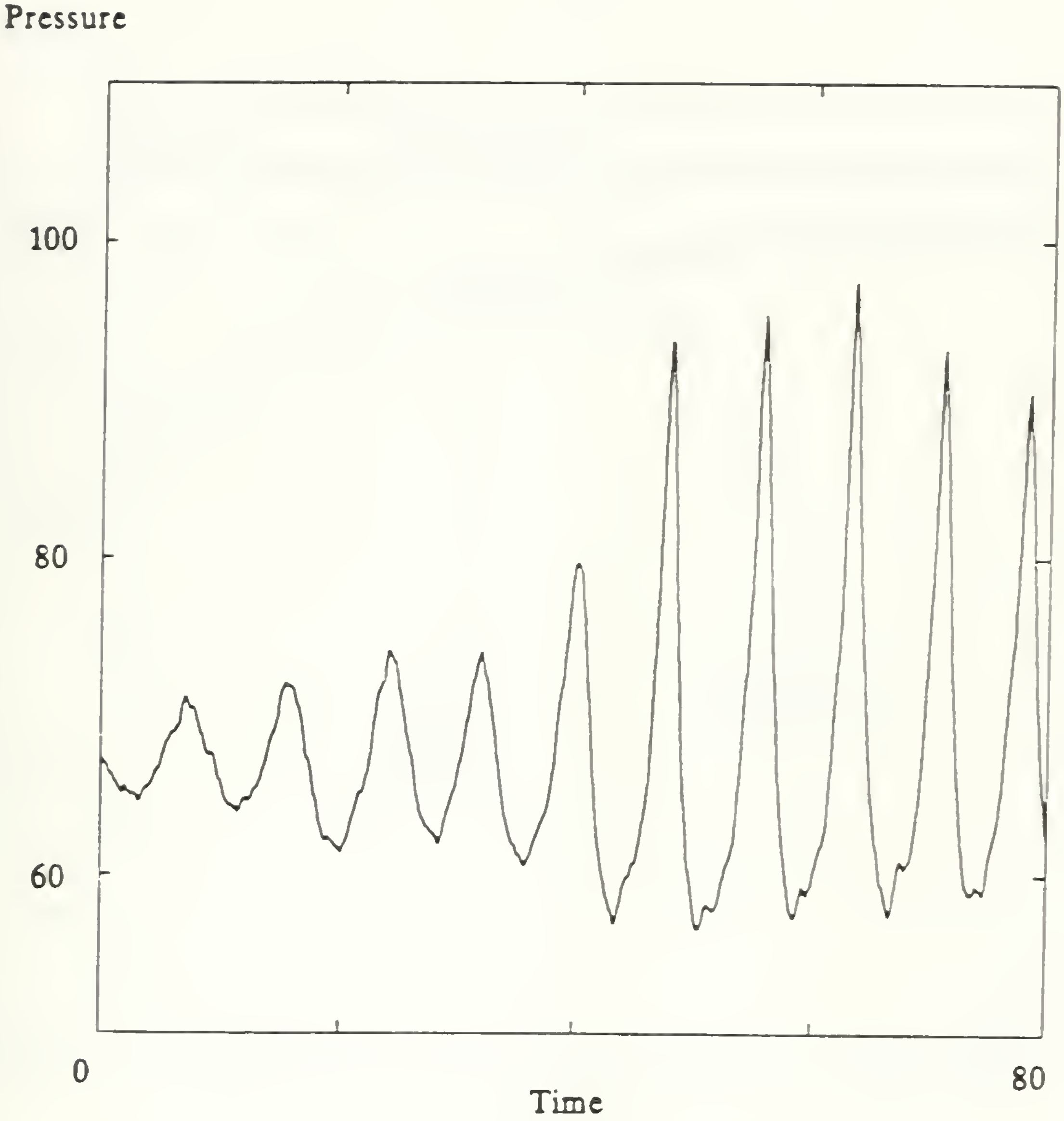

Fig. 2b. A 1D Unstable Computation. *A plot of pressure behind the shock initiating the detonation vs. time for the data described in [11, pp. 18-19]. The reaction zone was initialized with length 1.75. The ahead state has* $p = 1, u = 0, \rho = 1$. $q = 50, E = 50, \gamma = 1.2, k = 206$. *The speed of the initialized wave is 1.265 times the CJ wave speed for the ahead state. Grid spacing is 0.05. The results are similar to those in [6] and [11].*

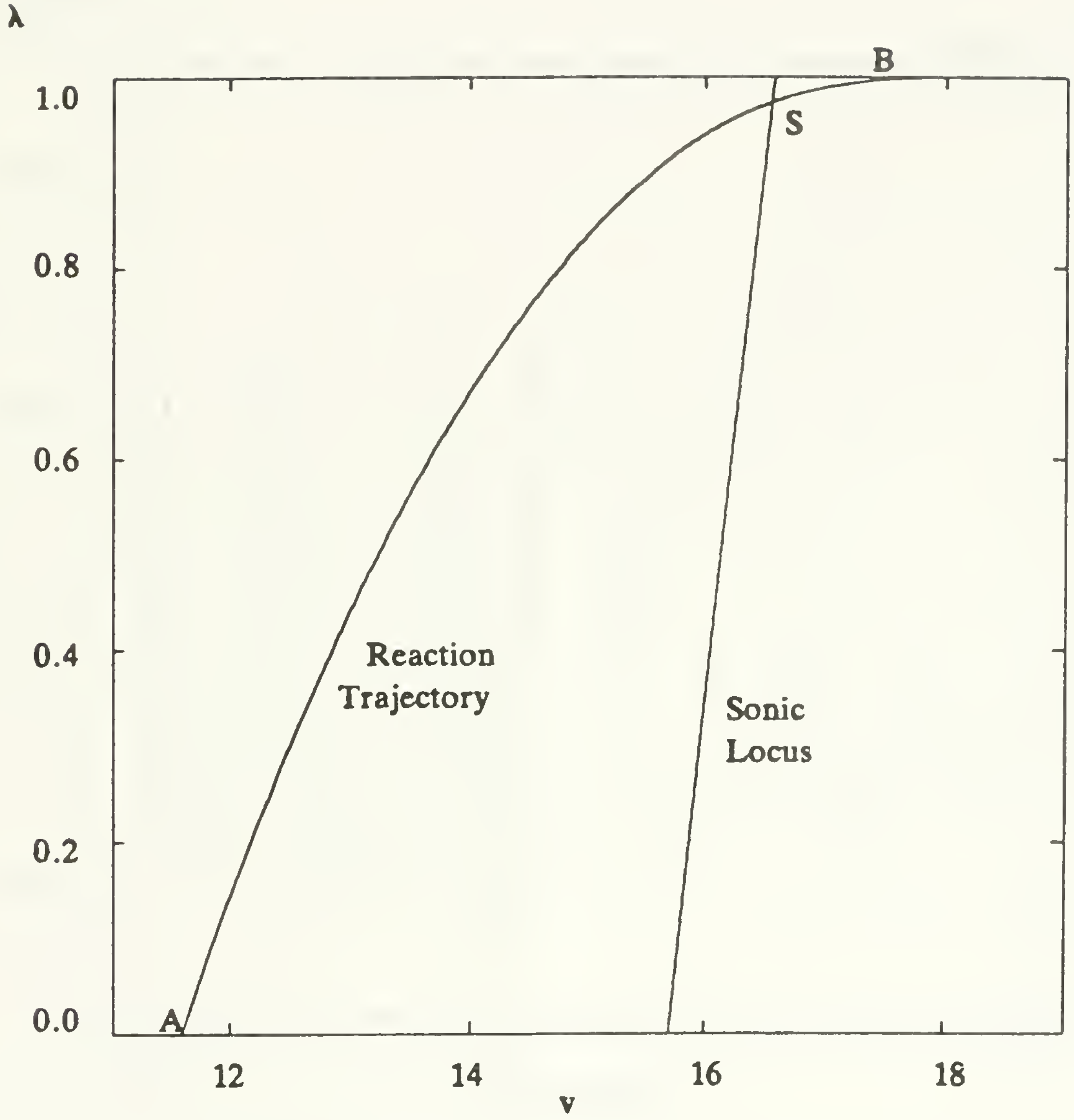

Fig. 3a. Phase Plane Portrait of the Reaction using Jones' Equations. *A plot of the trajectory through the sonic point (S) in the* v − λ *plane for the runs in the following figures when the radius of curvature is 50 times the reaction zone length. The sonic locus is also shown.* A *corresponds to the point behind the initiating shock wave while* B *represents the termination of the the reaction as a weak detonation.*

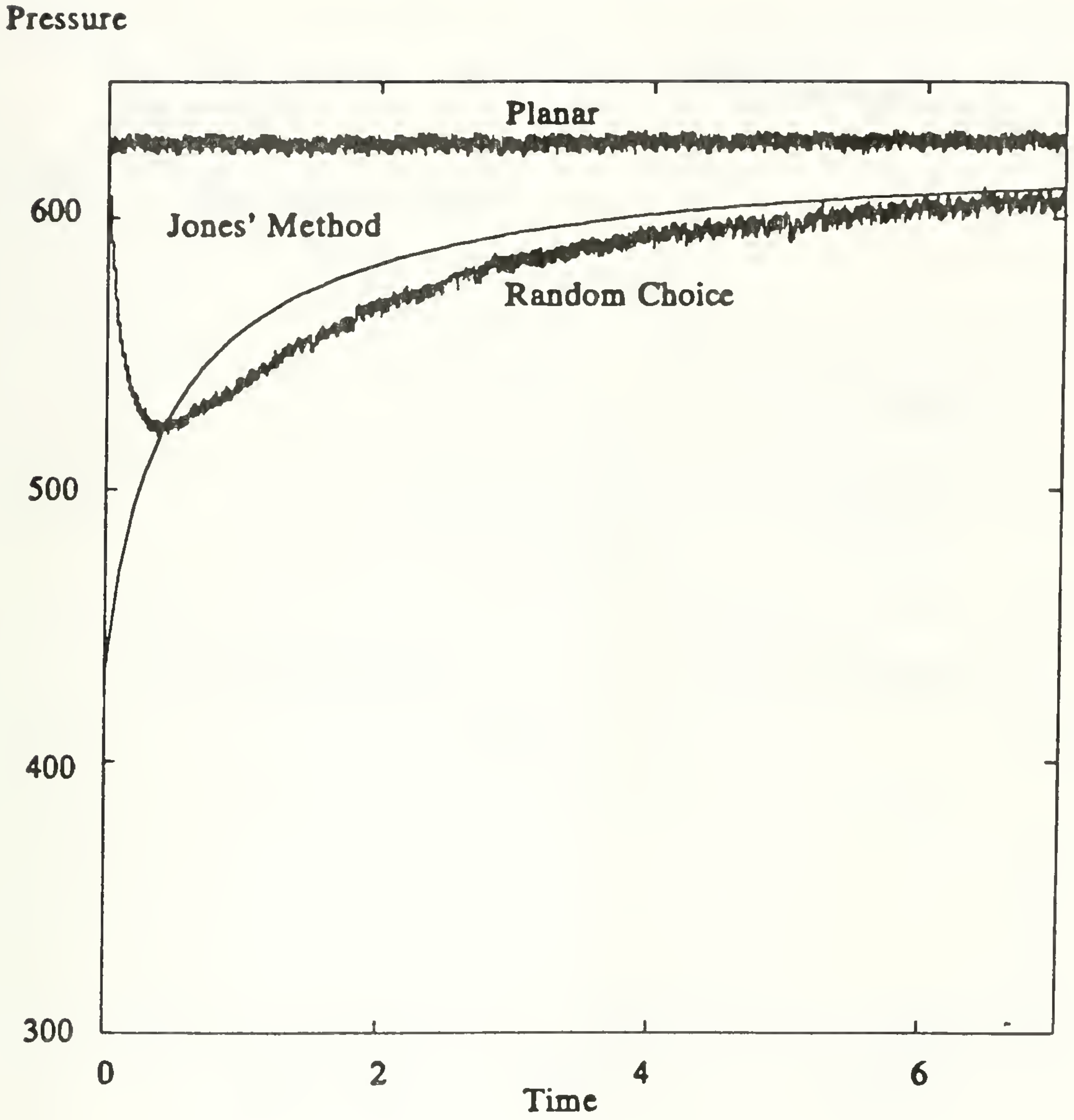

Fig. 4a. Effect of Curvature on Pressure behind the Initiating Shock. *A plot of pressure vs. time for planar and cylindrical computations using the random choice method of §2 and the solution to Jones' equations where the radius of curvature is assumed to be the same as for the cylindrical run by random choice. The error bars show the range of values over each 100 time steps for the random choice calculations. The ahead state has* $p = 300$, $u = 0$, $\rho = 1.4$. *The reaction zone has length 1,* $q = 300$, $T_c = 215$, $\gamma = 1.1$, $E = 100$ *and grid spacing 0.01.*

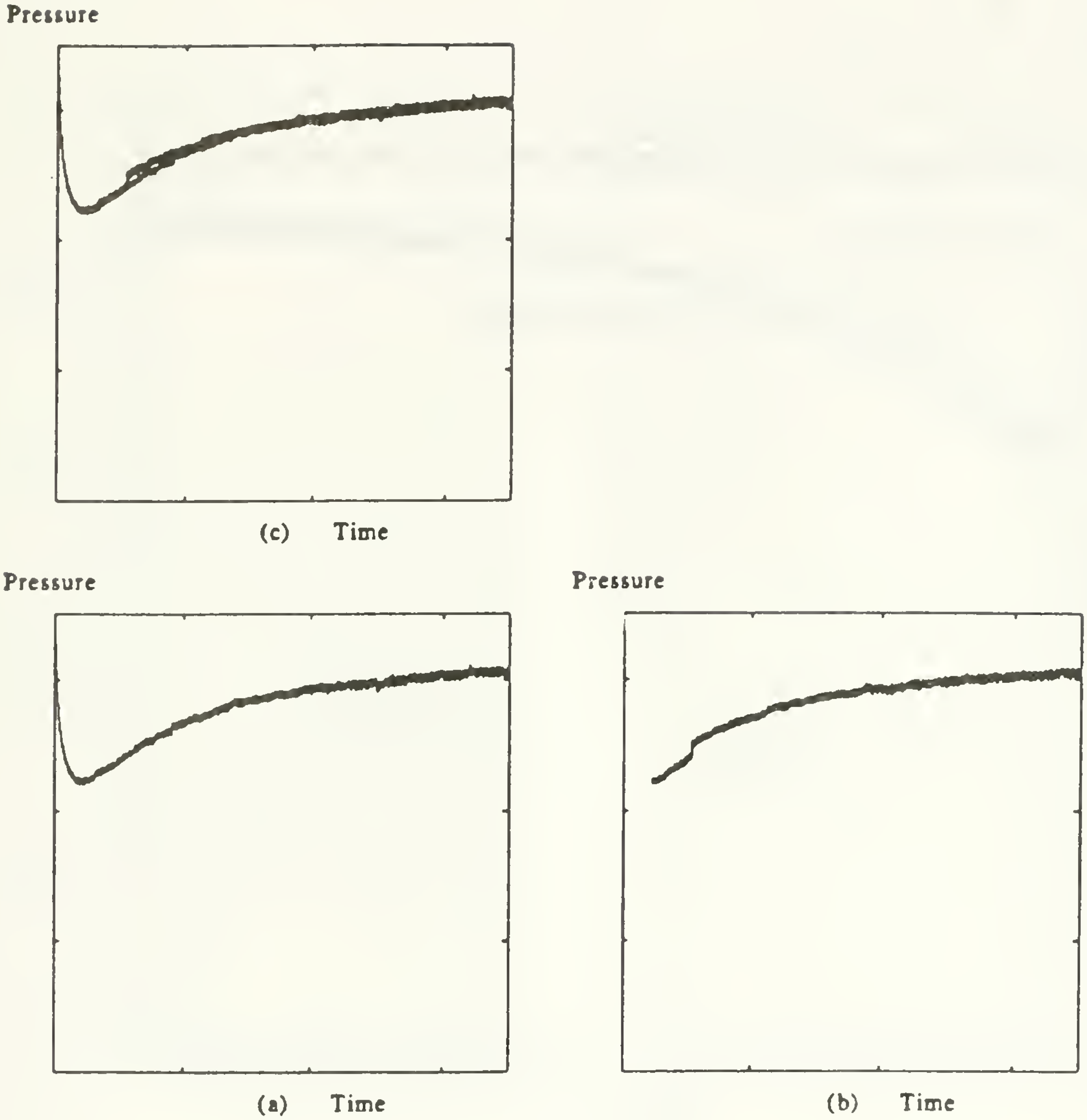

Fig. 4b. Comparison of Initializations. *The panels above show plots of pressure behind the initiating shock as a function of time for the same cylindrically expanding detonation problem as in* Fig. 4a *using the planar steady state initialization (a) and initialization by solution to Jones's method at a small radius (b). These two plots are superimposed in (c).*

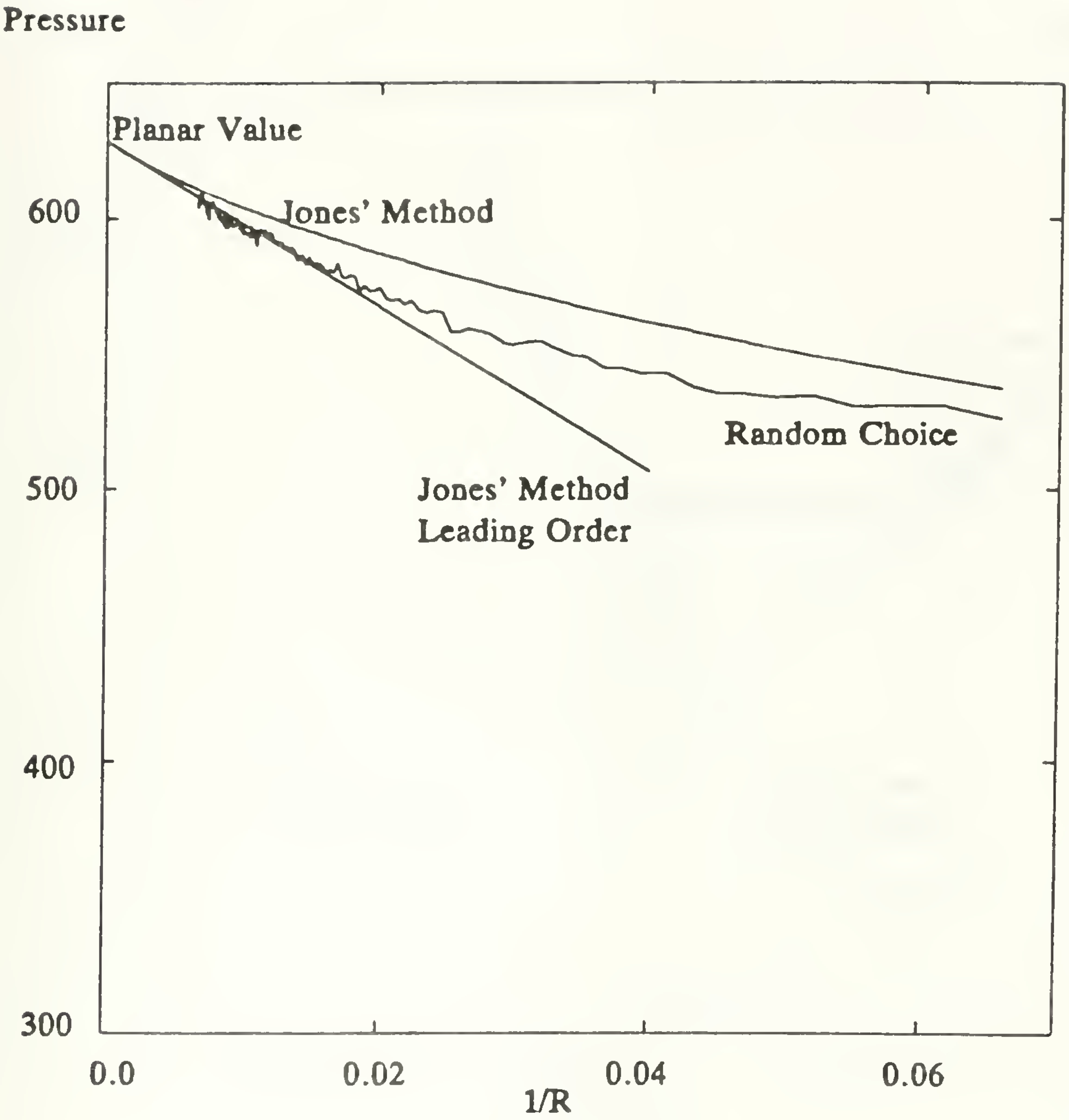

Fig. 4c. First Order Corrections to Pressure. *Pressure behind the initiating shock wave is plotted against inverse radius for the cylindrical computations of* Fig. 4a. *Also shown is the leading order correction predicted by solving Jones' equations for very large radii.*

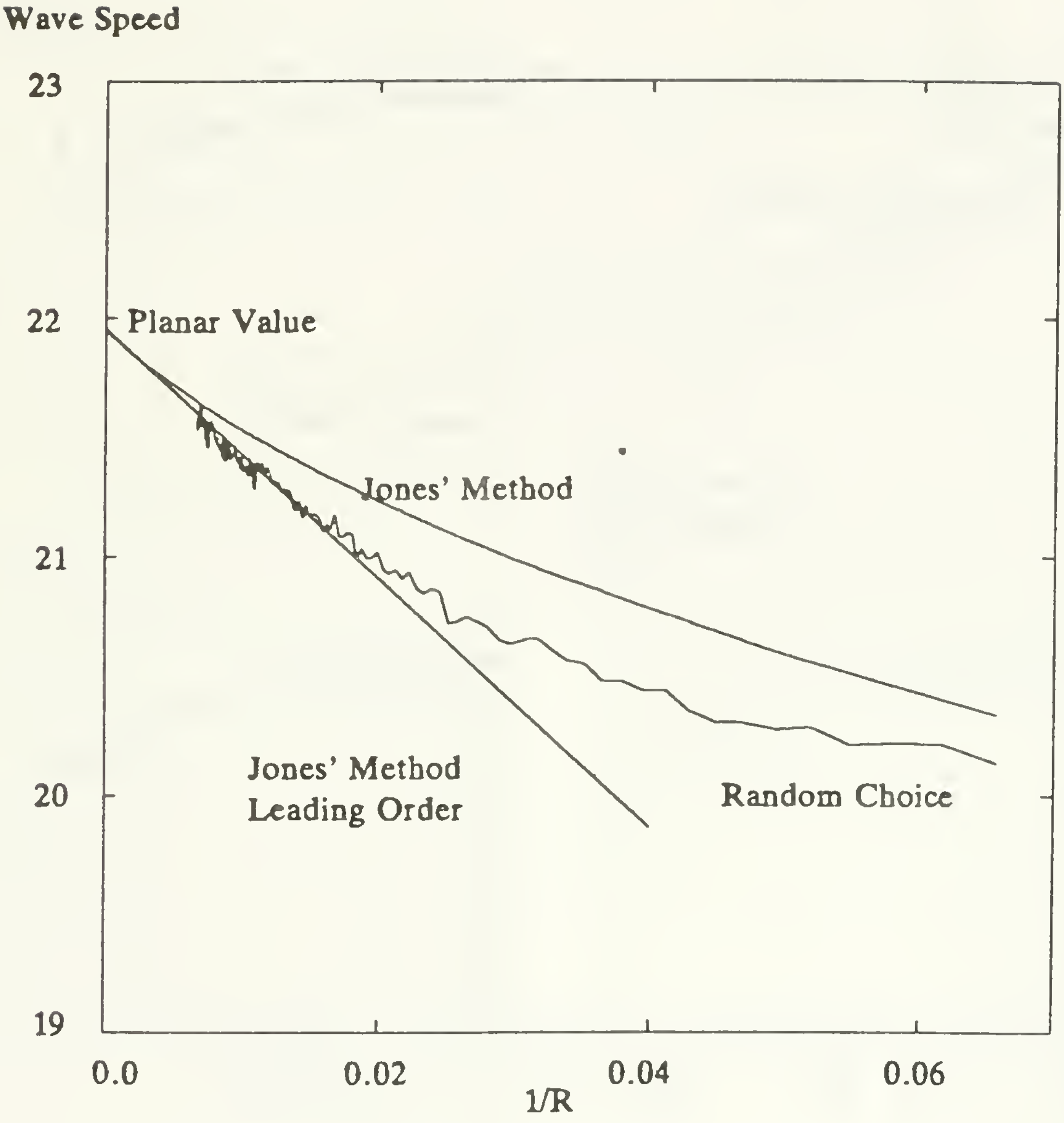

Fig. 4d. First Order Corrections to Wave Speed. *A plot of wave speed vs. inverse radius is shown corresponding to* Fig. 4c.

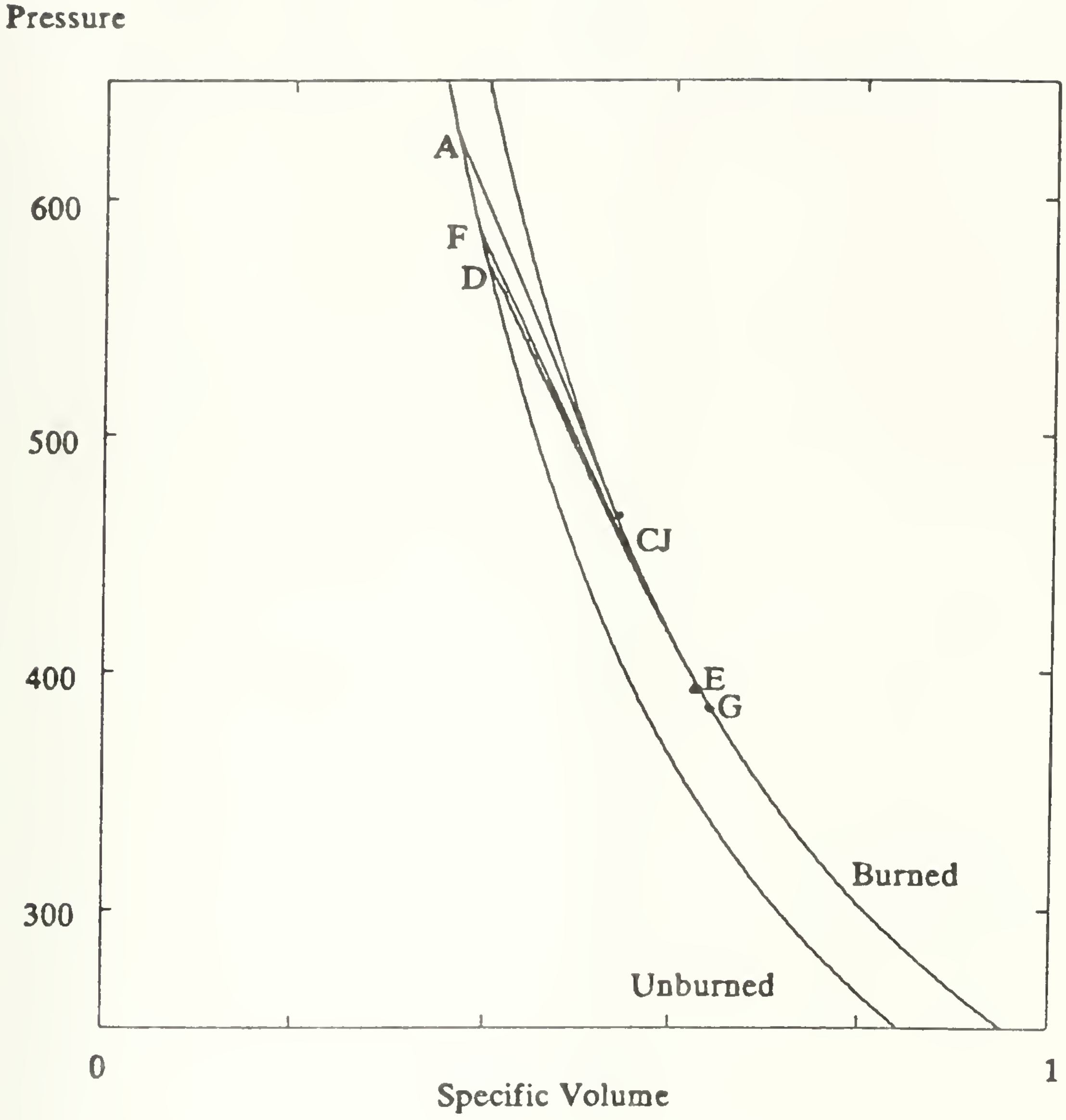

Fig. 4e. Effect of Curvature on the Hugoniot Diagram. *Pressure is plotted against specific volume for the calculations used in* Figs. 4a-d. *The unburned and burned Hugoniot curves are presented as well as the path through the reaction zone for a planar detonation (from* A *to* CJ*) and cylindrical detonations where the radius of curvature is approximately 50 times the reaction zone length by the random choice method (from* D *to* E*) and by Jones's method (from* F *to* G*). The pressure jump at the front is reduced by 12.5-17.5% by the curvature.*

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